IUCLID 5
Guidance and Support

Installation Guide for IUCLID 5 Version 5.3
Stand-alone Application

Installer for Microsoft® Windows®

August 2011

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http://echa.europa.eu.
http://europa.eu.

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Table of Contents

1. Introduction 1
1.1. Hardware requirements 1
1.2. Software requirements 1
2. Making a fresh installation of IUCLID 5 2
2.1. Installation of software required by IUCLID 5 2
2.1.1. Installation of Java 2
2.1.2. Installation of PostgreSQL 4
2.2. Installation of IUCLID 5 8
3. Upgrade 13
3.1. Upgrading from a previous version of IUCLID 5.3 to the latest version of IUCLID 5.3 13
3.1.1. Launching the installer 13
3.1.2. Installer option Upgrade from IUCLID 5.3.0 to 5.3.1 13
3.1.3. Destination folder for the installation 14
3.1.4. Installation of IUCLID 5.3.1 application files 15
3.1.5. Starting IUCLID 5 16
3.2. Upgrade from IUCLID 5.2 to IUCLID 5.3 16
3.2.1. Launching the installer 17
3.2.2. Installer option Upgrade to IUCLID 5.3 17
3.2.3. Destination folder for the installation 18
3.2.4. Installation of IUCLID 5.3.1 application files 19
3.2.5. The migration tool 20
3.2.6. Starting IUCLID 5 21
3.3. Upgrading from IUCLID 5.0 / 5.1 to IUCLID 5.3 22
3.3.1. Migration of data to IUCLID 5.3 from a previous version 22
3.3.2. Database configuration for running IUCLID 5.3 and a previous version at the same time 22
3.3.3. IUCLID 5.0 / 5.1 was installed using the setup-kit 22
3.3.4. IUCLID 5.0 / 5.1 was installed manually 22
4. Initialisation of an installation of IUCLID 5 24
4.1. Starting IUCLID 5 24
4.2. First steps wizard 24
4.3. User management 30
5. Un-installation of IUCLID 5 31
A. Tips on launching the installer and access rights 32

Chapter 1. Introduction

IUCLID 5 can be installed either as a stand-alone application, or in a multi-user environment that uses client-server architecture. This document describes how to use a dedicated installer to install IUCLID 5 as a stand-alone application on a computer running Microsoft® Windows® (hereafter referred to as Windows). The installer can be downloaded from the IUCLID 5 web site. The installation is performed by ensuring that the prerequisite software is installed, then running the installer; typically by double clicking on it. If the instructions in this document are followed with care, no prior specialist knowledge is required of either the IUCLID 5 software, or the software components required to run it.

If you encounter any problems during the installation that cannot be solved using information in this manual, or the documentation of third party softwares; before contacting the ECHA Helpdesk, please try the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.

1.1. Hardware requirements

The following requirements are provided as only a guide.

- At least 1 GB of mother board RAM (2 GB for Windows Vista®)
- Pentium Core 2 duo or equivalent

An installation of IUCLID 5 will most likely run on a lower specified machine but the performance might not be satisfactory. The requirements depend in part on the version of Windows and the IUCLID plugins that are in use. For example, using the Query Tool plugin will increase the resources required to obtain a reasonable running speed; especially on a large database.

1.2. Software requirements

The software prerequisites for the installation are as follows:

- Windows with access to a user account that can run the installer and create the required directories.
- Java - J2SE Runtime Environment v6
- Database - PostgreSQL 8.2, 8.3, 8.4 (recommended) or 9.
- The Windows installer for IUCLID 5.3 that can be downloaded without charge from the IUCLID 5 web site.
- Once you have completed the installation of IUCLID 5, you should test it by starting and configuring it. The configuration requires access to at least a legal entity file (LEOX). The creation of a LEOX is described on the IUCLID 5 web site where the installation software is published. In addition, it is recommended to upload a set of reference substances and the EC inventory. These are also available from the web site at which the IUCLID 5 software is published.

Tip

Time and IT resources can be saved by importing into IUCLID only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set*, a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

Chapter 2. Making a fresh installation of IUCLID 5

If Java and PostgreSQL are already installed as required, go straight to section Section 2.2, “Installation of IUCLID 5”.

2.1. Installation of software required by IUCLID 5

The installation of third party software is described by the respective publishers. Please refer to their web sites for full instructions.

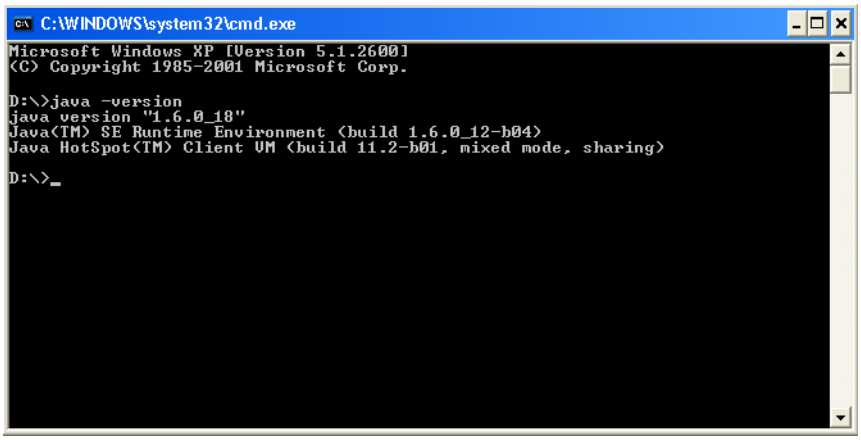
2.1.1. Installation of Java

1. Verify whether Java (JRE) of the correct version is installed on the computer to which IUCLID will be installed:

   Open a command prompt (Start # Run… # Open: cmd). At the command prompt, enter the following:

   ```
   java -version
   ```

   Figure 2.1. Check version of Java

   
   C:\WINDOWS\system32\cmd.exe
Microsoft Windows XP [Version 5.1.2600]
(C) Copyright 1985-2001 Microsoft Corp.
D:\>java -version
java version "1.6.0_18"
Java(TM) SE Runtime Environment (build 1.6.0_12-b04)
Java HotSpot(TM) Client VM (build 11.2-b01, mixed mode, sharing)
D:\>

2. If a message similar to the one shown in the screen shot above is not shown, or the version of Java is not 1.6 or higher, install the latest version. It can be downloaded from the Sun site at www.java.com.

Figure 2.2. Installation wizard for Java

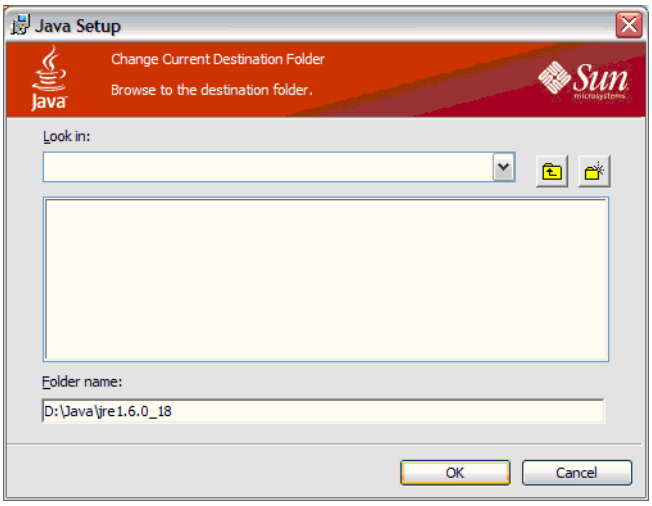


Figure 2.3. Choose installation directory for Java

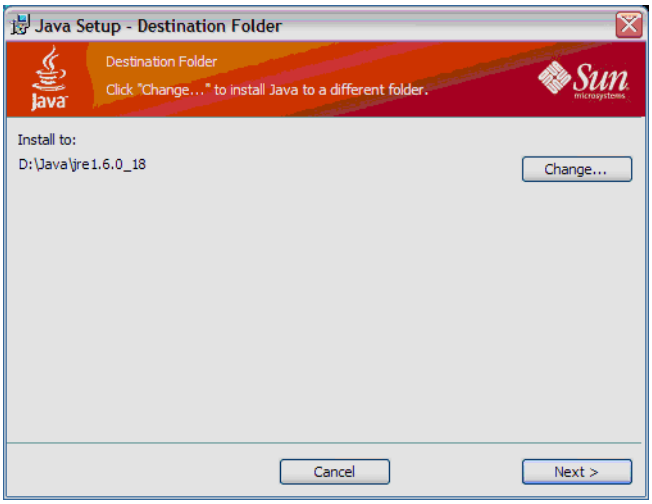
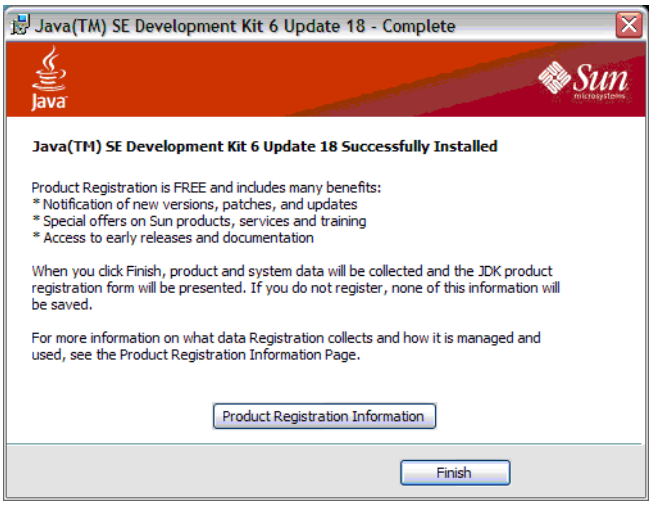


Figure 2.4. Installation of Java is complete


Java(TM) SE Development Kit 6 Update 18 - Complete
Java
Sun
Java(TM) SE Development Kit 6 Update 18 Successfully Installed
Product Registration is FREE and includes many benefits:
* Notification of new versions, patches, and updates
* Special offers on Sun products, services and training
* Access to early releases and documentation
When you click Finish, product and system data will be collected and the JDK product registration form will be presented. If you do not register, none of this information will be saved.
For more information on what data Registration collects and how it is managed and used, see the Product Registration Information Page.
Product Registration Information
Finish

2.1.2. Installation of PostgreSQL

If either version 8.2, 8.3 or 8.4 of PostgreSQL is already installed and running as a service with a user `postgres`, the existing installation can be used. There is no need to upgrade to 9, although 9 is supported. If PostgreSQL is not already installed on the computer, or you would like to upgrade to 9, download PostgreSQL 9 from the site www.postgresql.org/download and install it. The web site of PostgreSQL offers a range of alternative ways to download and install the PostgreSQL software. The screen shots shown below show the use of the *one click installer* available from the PostgreSQL web site. An example of the file name of the installer is *postgresql-9.0.4-1-windows.exe*.

The default fresh installation of PostgreSQL, made using the *one click installer*, automatically starts PostgreSQL as a service, creates the user `postgres` if necessary, and supplies administration tools (e.g. pgAdmin III) that can be used to create the database. If the installer creates the superuser `postgres`, you will have to create a password for it, as shown in the figure below, and enter it later into the configuration file for IUCLID 5.

Figure 2.5. Installer for PostgreSQL

Figure 2.6. Installation directory for PostgreSQL

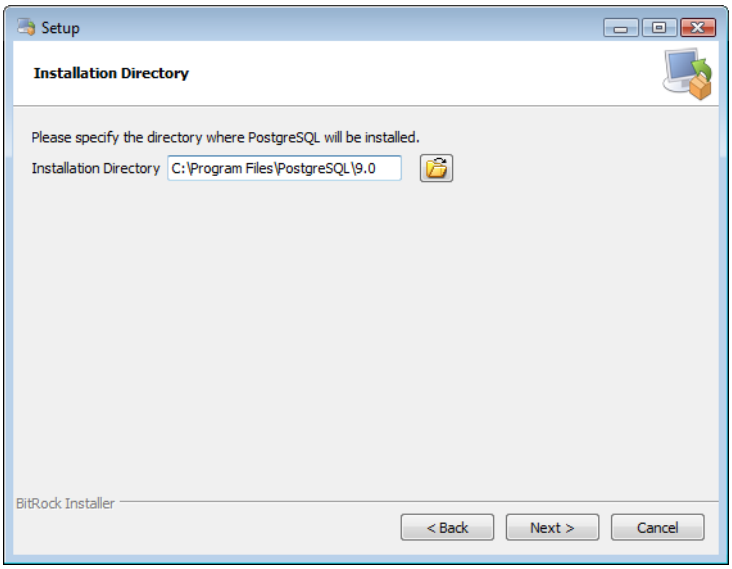


Figure 2.7. Data directory for PostgreSQL

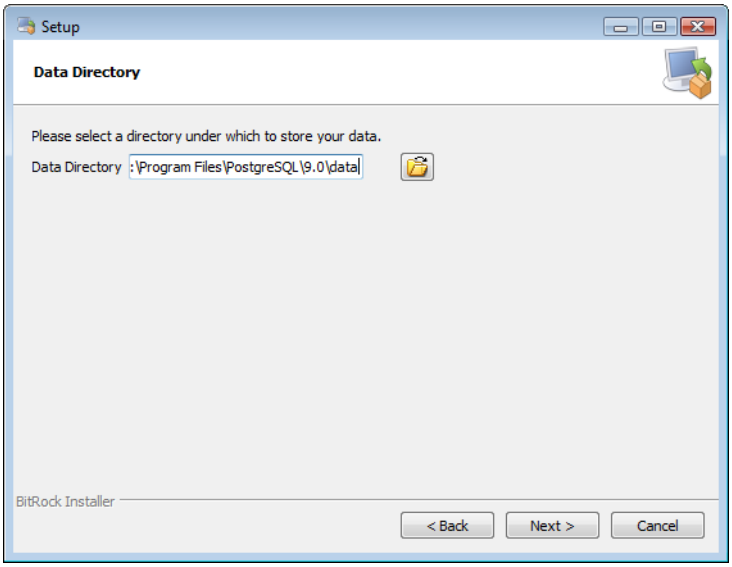


Figure 2.8. Password for the database superuser (postgres) and the Windows service account (postgres)

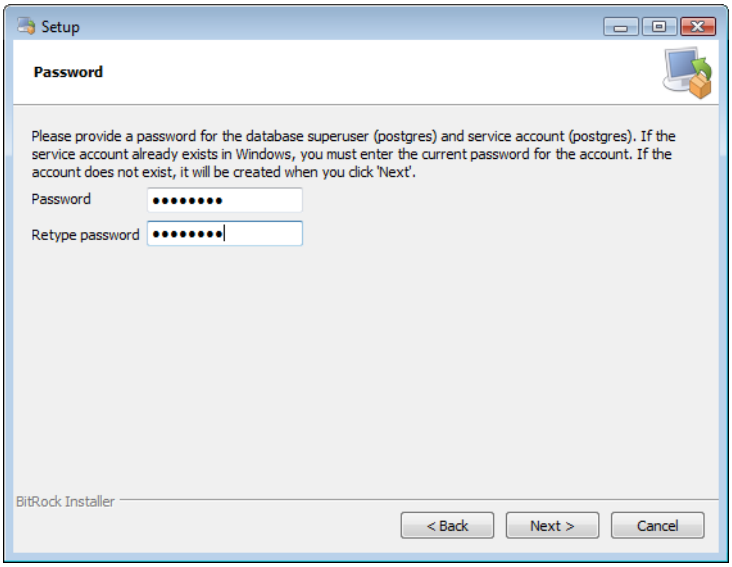

Setup
Password
Please provide a password for the database superuser (postgres) and service account (postgres). If the service account already exists in Windows, you must enter the current password for the account. If the account does not exist, it will be created when you click 'Next'.
Password
Retype password
BitRock Installer
< Back
Next >
Cancel

Figure 2.9. Port number for PostgreSQL

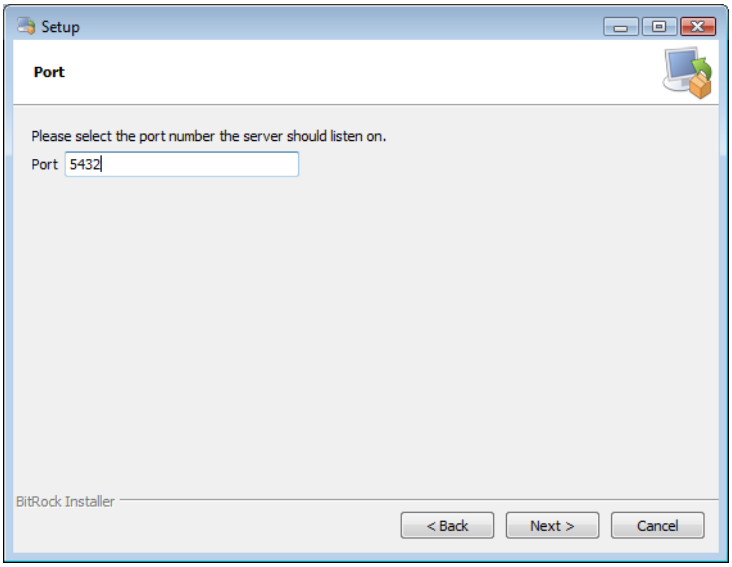


Figure 2.10. Set the default locale for PostgreSQL

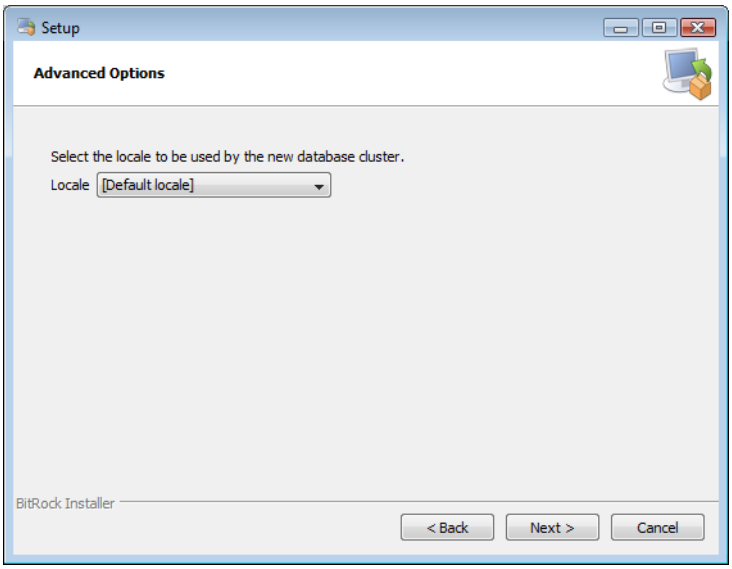


Figure 2.11. Confirm installation of PostgreSQL

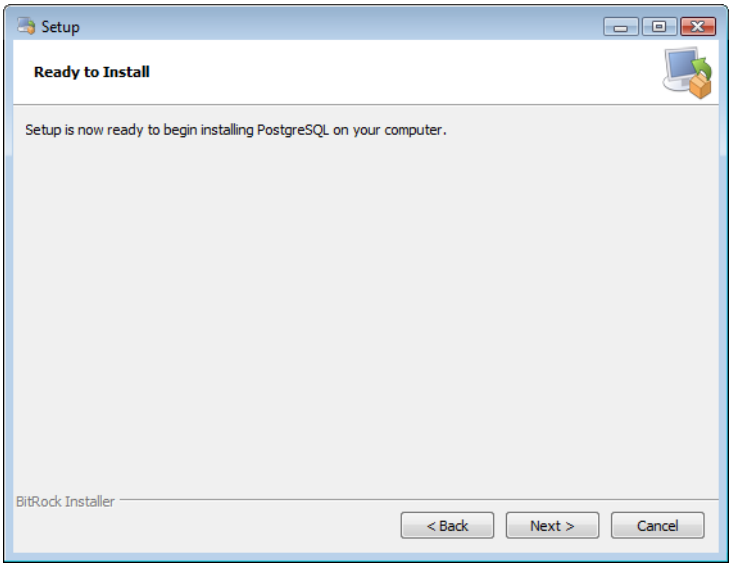


Figure 2.12. Installation of PostgreSQL in progress

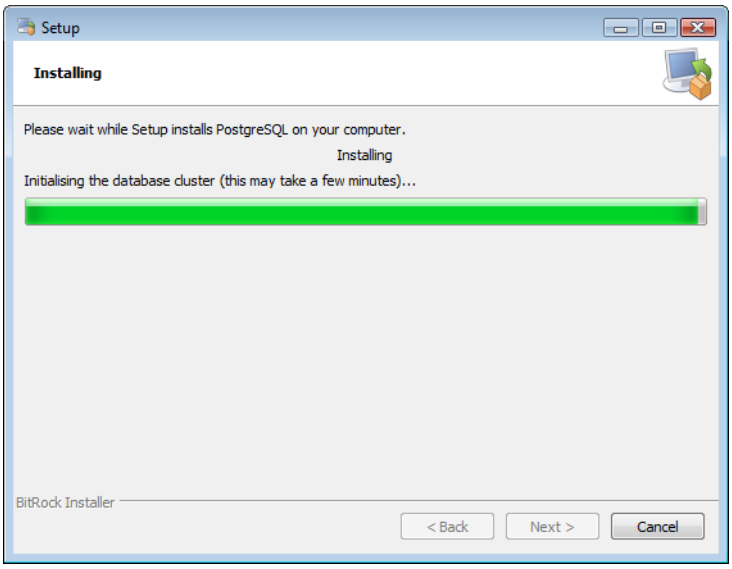


Figure 2.13. Installation of PostgreSQL complete

Setup
Completing the PostgreSQL Setup Wizard
Setup has finished installing PostgreSQL on your computer.
Launch Stack Builder at exit?
Stack Builder may be used to download and install additional tools, drivers and applications to complement your PostgreSQL installation.
PostgreSQL
Packaged by:
EnterpriseDB
The Enterprise PostgreSQL Company
< Back
Finish
Cancel

2.2. Installation of IUCLID 5

After downloading the Windows installer installation package, unzip its content to a convenient folder.

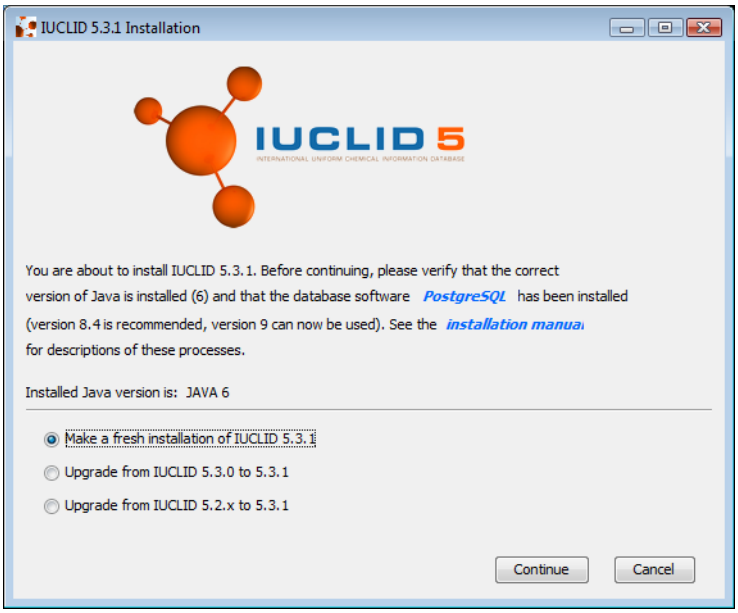
The installer is supplied as an executable Java file named `iuclid5_install.jar`. It can be launched either by double-clicking on the file, or by running it from the command line, as you would a script. Bear in mind that the user account under which the installer is run, must have permission to write to the folder in which IUCLID 5.3 will be installed.

If you experience problems in running the installer, for a possible solution, see Appendix A, *Tips on launching the installer and access rights* later in this document.

The first screen of the installer offers the choice between a fresh installation of IUCLID 5.3.1, or an upgrade to IUCLID 5.3.1, from either IUCLID 5.3.0 or IUCLID 5.2. To upgrade, please refer to the section in this manual, Upgrade. The texts in blue are links to the web site of PostgreSQL and the installation manuals on the IUCLID web site.

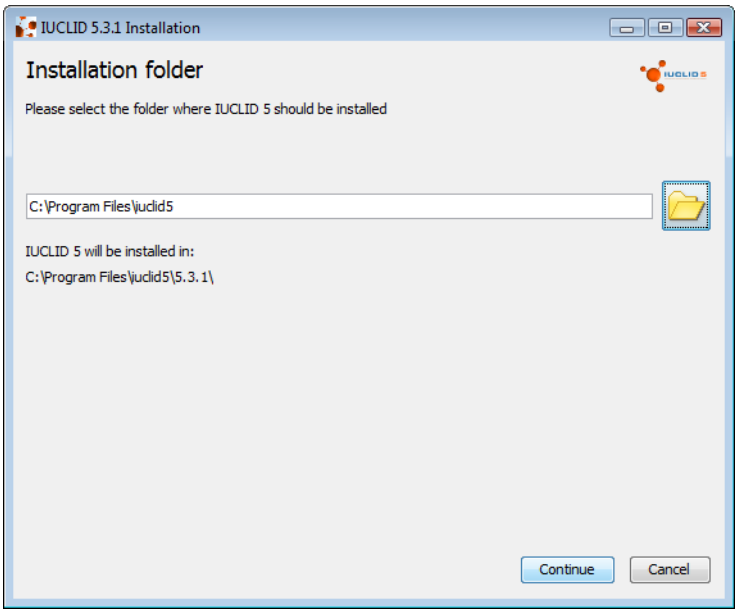
For a fresh installation of IUCLID 5.3 with an empty database, select the option Make a fresh installation of IUCLID 5.3.1, then click on Continue.

Figure 2.14. Install IUCLID 5.3 with no upgrade


IUCLID 5.3.1 Installation
IUCLID 5
You are about to install IUCLID 5.3.1. Before continuing, please verify that the correct
version of Java is installed (6) and that the database software PostgreSQL has been installed
(version 8.4 is recommended, version 9 can now be used). See the installation manual
for descriptions of these processes.
Installed Java version is: JAVA 6
Make a fresh installation of IUCLID 5.3.1
Upgrade from IUCLID 5.3.0 to 5.3.1
Upgrade from IUCLID 5.2.x to 5.3.1
Continue
Cancel

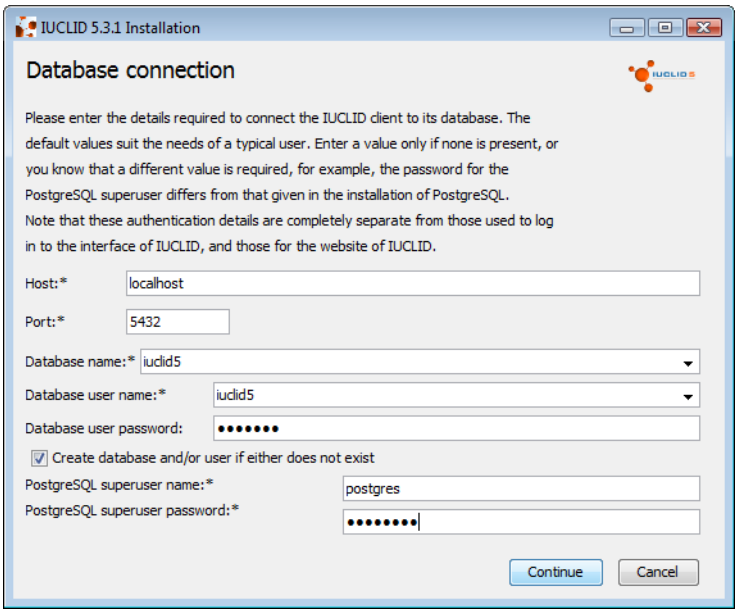
The next page of the installer allows you to change the parent folder of the installation folder for IUCLID 5.3. The software will be installed in a folder named `5.3.1` that is created inside the parent folder. For example, in the screenshot shown below, the path and name of the parent folder are `C:\Program Files\iuclid5`. Ensure that the user account in Windows used to run the installer has the permission to write to the destination folder.

Figure 2.15. Destination folder



The second screen of the installer helps to set-up the connection to the PostgreSQL database. The default values suit the needs of a typical user, so unless values are missing, or you know that different values are required, leave the default values in place and click on Continue.

Figure 2.16. Database connection


IUCLID 5.3.1 Installation
Database connection
Please enter the details required to connect the IUCLID client to its database. The default values suit the needs of a typical user. Enter a value only if none is present, or you know that a different value is required, for example, the password for the PostgreSQL superuser differs from that given in the installation of PostgreSQL.
Note that these authentication details are completely separate from those used to log in to the interface of IUCLID, and those for the website of IUCLID.
Host:*
localhost
Port:*
5432
Database name:*
iuclid5
Database user name:*
iuclid5
Database user password:
Create database and/or user if either does not exist
PostgreSQL superuser name:*
postgres
PostgreSQL superuser password:*
Continue
Cancel

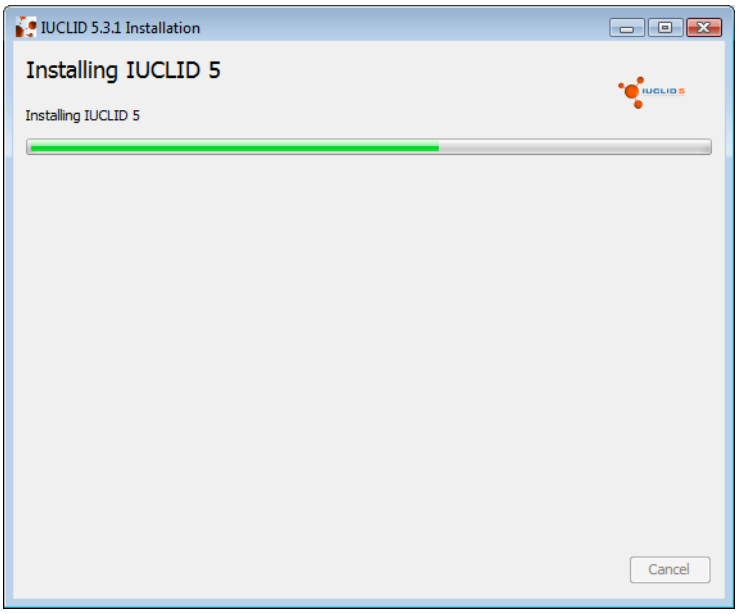
If the following error message is displayed *password authentication failed for user postgres*, try again after entering the password of the superuser for PostgreSQL that was entered during the installation of PostgreSQL.

Figure 2.17. Wrong password

If either of the two error messages *Cannot create destination folder* or *Access denied* are given, for a possible solution, see Appendix A, *Tips on launching the installer and access rights* later in this document.

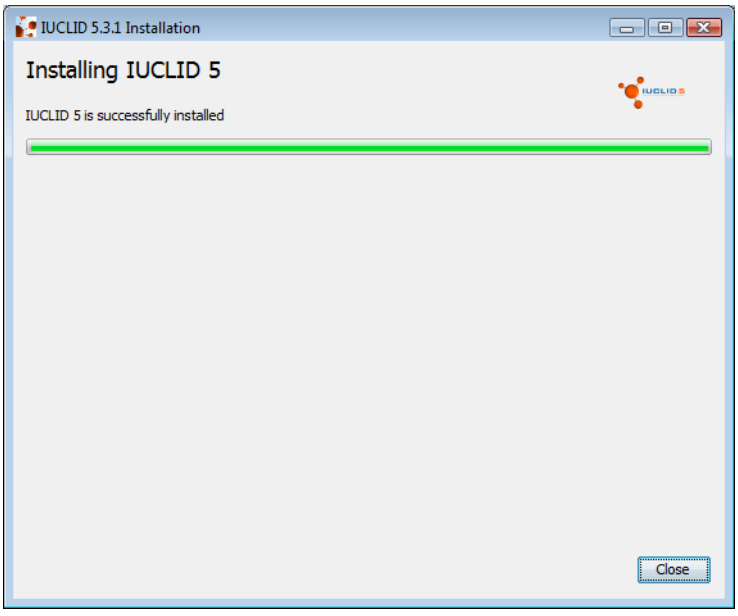
The actual installation process will take a few seconds.

Figure 2.18. Installing IUCLID 5



When the installer has finished installing the application, you can Close the installer.

Figure 2.19. Successful installation



A new shortcut has been created automatically on your Desktop. The shortcut points to the file `iuclid5.cmd` that is included in the installation directory. If no shortcut is created, see Appendix A, *Tips on launching the installer and access rights* for possible reasons. It is possible to create a shortcut manually. The next step is to initialise the installation, as described in Chapter 4, *Initialisation of an installation of IUCLID 5* of this document. After that, if you have data that was exported from IUCLID using its built-in back-up/restore functionality, it can be imported into the fresh installation of IUCLID 5.3.

Figure 2.20. Shortcut to IUCLID 5

Chapter 3. Upgrade

This chapter describes how to upgrade a previous version of IUCLID 5 to the most recent version of IUCLID 5.3. Dependent upon the version of IUCLID 5 that is being upgraded, there are three main scenarios in the upgrade process: upgrade from a previous version of 5.3, upgrade from any version of 5.2, and upgrade from 5.0 or 5.1. These are each described in a dedicated sub-section of this chapter. In all scenarios, before starting the upgrade, it is important to back-up the database. Use the built-in back-up functionality of IUCLID, and/or the back-up functionality of the database. Making only a copy of the file system on which IUCLID is installed is not recommended as a means of backing-up.

3.1. Upgrading from a previous version of IUCLID 5.3 to the latest version of IUCLID 5.3

This section applies only to users who have an existing IUCLID 5.3 installation. If you are unsure which version you are currently using, you can read it from within the interface of IUCLID 5. Start IUCLID 5, log-in, then click 'Help' and select 'About'.

Upgrading from a previous version of IUCLID 5.3 to the latest version of IUCLID 5.3 does not require a separate migration step. On starting the new version of IUCLID 5.3, it can connect to the previous database. The installer provides a simple way of performing the upgrade, as described in the sections that follow.

1. Back-up the database. Use the built-in back-up functionality of IUCLID, and/or the back-up function of PostgreSQL.

2. Run the installer, select the upgrade option that is appropriate for your system, and then proceed with the installation.

Important

The upgrade functionality of the Windows installer can be used only if IUCLID 5.3 was installed using the Windows installer.

For instructions on how to upgrade IUCLID 5.3 without the Windows installer, please refer to the specific installation manual for your computer set-up.

3.1.1. Launching the installer

After downloading the Windows installer installation package, unzip its content to a convenient folder.

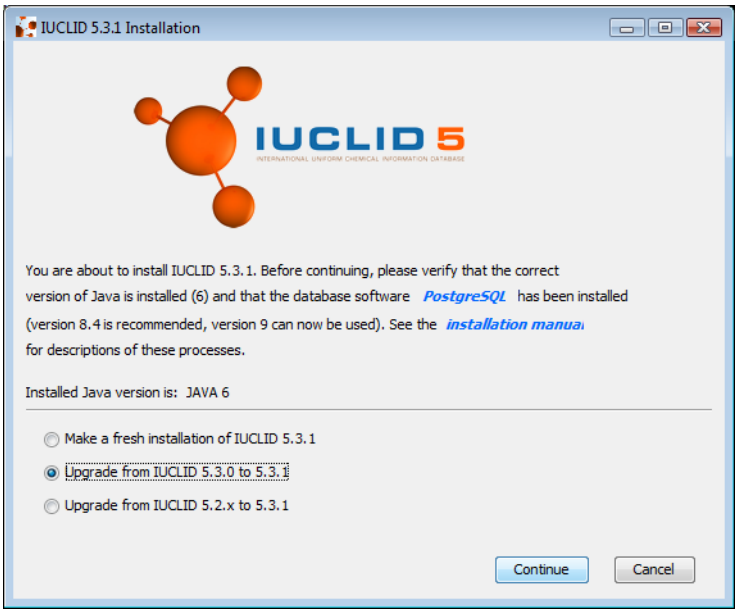
The installer is supplied as an executable Java file named `iuclid5_install.jar`. It can be launched either by double-clicking on the file, or by running it from the command line, as you would a script. Bear in mind, that the user account under which the installer is run, must have permission to write to the folder in which IUCLID will be installed.

If you experience problems in running the installer, for a possible solution, see Appendix A, *Tips on launching the installer and access rights* in the Appendix of this document.

3.1.2. Installer option *Upgrade from IUCLID 5.3.0 to 5.3.1*

On the first screen of the installer, select the option Upgrade from IUCLID 5.3.0 to 5.3.1, then click continue.

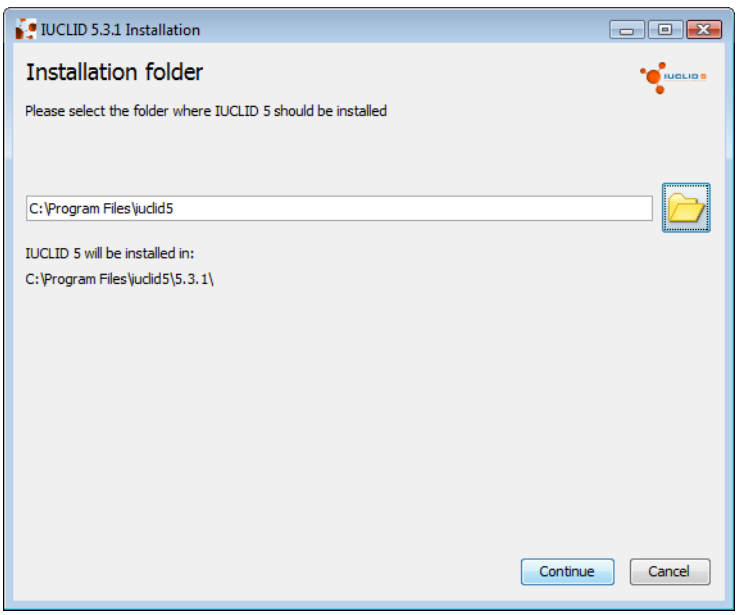
Figure 3.1. Upgrade from IUCLID 5.3.0 to 5.3.1


IUCLID 5.3.1 Installation
IUCLID 5
You are about to install IUCLID 5.3.1. Before continuing, please verify that the correct
version of Java is installed (6) and that the database software PostgreSQL has been installed
(version 8.4 is recommended, version 9 can now be used). See the installation manua
for descriptions of these processes.
Installed Java version is: JAVA 6
Make a fresh installation of IUCLID 5.3.1
Upgrade from IUCLID 5.3.0 to 5.3.1
Upgrade from IUCLID 5.2.x to 5.3.1
Continue
Cancel

3.1.3. Destination folder for the installation

The installer leaves the application files for IUCLID 5.3.0 in their installation folder, and creates a new installation folder for IUCLID 5.3.1. In the second step of the installer, the path to the installation folder of IUCLID 5.3.1 is entered. It can be either the default as shown in the screen shot below `C:\Program Files\iuclid5`, or you can enter a different value. The installer reads the database configuration parameters from the installation folder for IUCLID 5.3.0, and then copies them to the new installation.

Figure 3.2. Installation folder

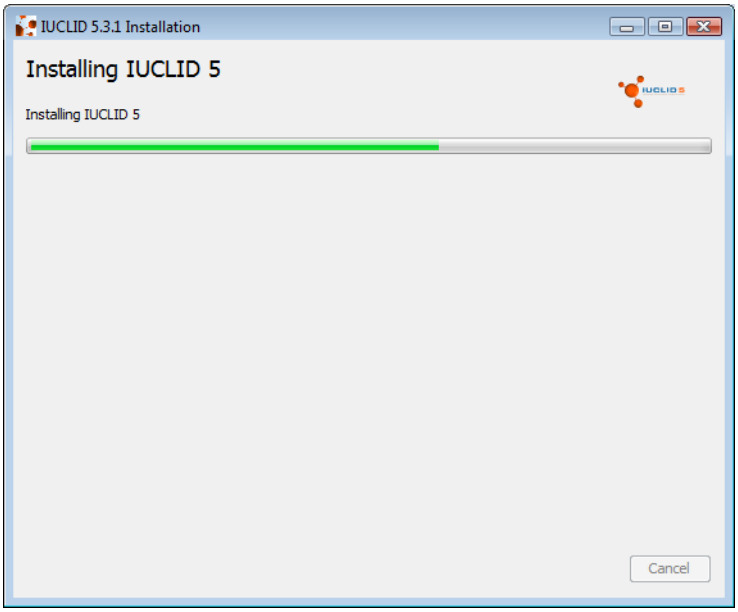


When you are sure that the values are correct, click Continue.

3.1.4. Installation of IUCLID 5.3.1 application files

The actual installation process will take a few seconds.

Figure 3.3. Installing IUCLID 5



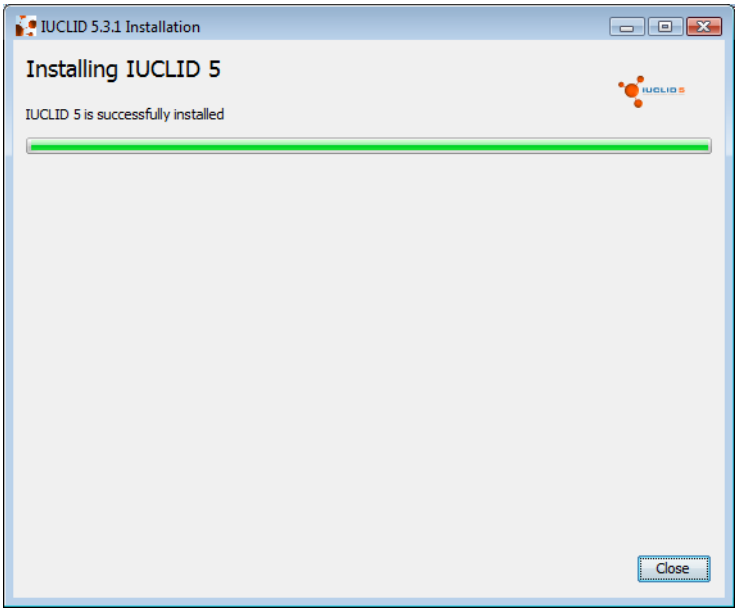
During the installation process, the following operations are performed:

- The new versions of the application files are copied to the installation folder of the new version.
- Plugins that had been installed in the previous version of IUCLID 5, are copied over to the new version of IUCLID 5, but only if they are compatible with the new version. The installer automatically detects whether a plugin is compatible. If a plugin is no longer visible in the user interface of IUCLID 5 after upgrading, visit the IUCLID web site at http://iuclid.eu to see whether a compatible version is available.
- The configuration files for the previous installation are copied to the new installation.
- A shortcut to IUCLID 5 is created on the desktop of the Windows account under which the installation is performed, as shown below.

Figure 3.4. Shortcut to IUCLID 5

After a successful upgrade from IUCLID 5.3.0 to 5.3.1, the following screen is shown.

Figure 3.5. IUCLID 5.3.1 is installed successfully



Click Close.

3.1.5. Starting IUCLID 5

You can now launch the newly installed IUCLID 5. Launch IUCLID 5 by double-clicking the icon that the installer created on your Desktop, as shown below. It is also possible to launch IUCLID 5 by running the file `iuclid5.cmd` that is included in the installation directory. The initialisation process is not required. All of the data that was present in the upgraded system should be present in the new system. Therefore, it should be possible to log in to any of the user accounts from the previous system.

Figure 3.6. Shortcut to IUCLID 5

3.2. Upgrade from IUCLID 5.2 to IUCLID 5.3

If you already have a working installation of IUCLID 5.2, the installer provides a simple way of upgrading it, as described in the sections that follow. The upgrade process consists of the following three parts:

1. Back-up the database. Use the built-in back-up functionality of IUCLID, and/or the back-up function of PostgreSQL.

2. Run the installer, select the upgrade option and proceed with the installation.

3. Run the migration tool. This is a script that is supplied along with the installer. It migrates existing IUCLID data into the new format for IUCLID 5.3. IUCLID cannot be started until the migration tool has been successfully run.

Important

The upgrade functionality of the Windows installer can be used only if IUCLID 5.2 was installed using the Windows installer.

For instructions on how to carry out the installation of IUCLID 5.3 without the Windows installer, please refer to the specific installation manual for your computer set-up.

3.2.1. Launching the installer

After downloading the Windows installer installation package, unzip its content to a convenient folder.

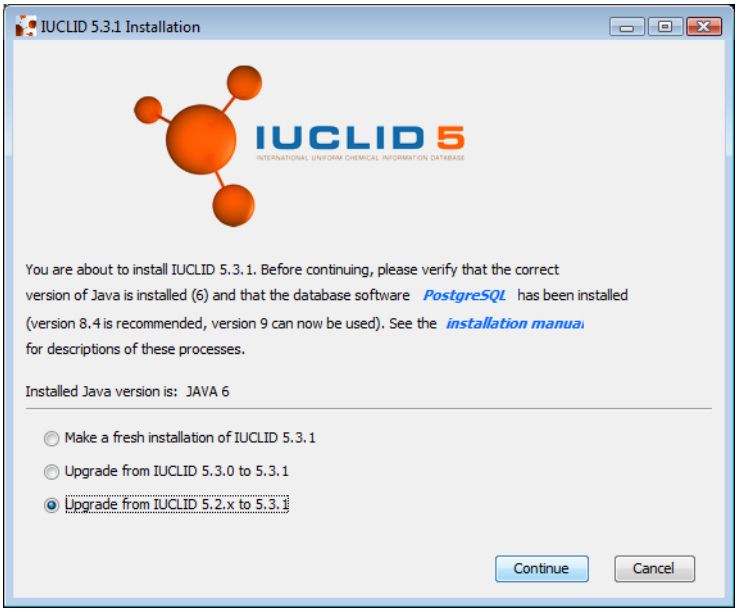
The installer is supplied as an executable Java file named `iuclid5_install.jar`. It can be launched either by double-clicking on the file, or by running it from the command line, as you would a script. Bear in mind, that the user account under which the installer is run, must have permission to write to the folder in which IUCLID will be installed.

If you experience problems in running the installer, for a possible solution, see Appendix A, *Tips on launching the installer and access rights* in the Appendix of this document.

3.2.2. Installer option *Upgrade to IUCLID 5.3*

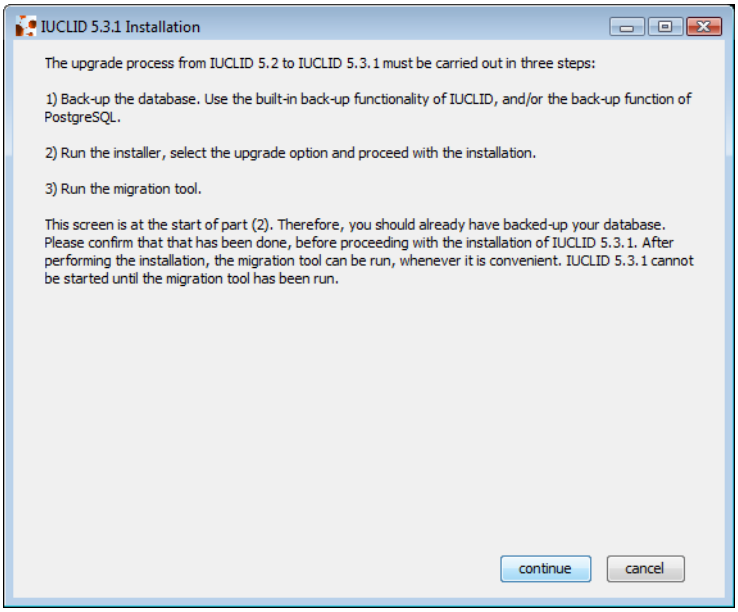
On the first screen of the installer, select the option Upgrade from IUCLID 5.2.x to 5.3.1, then click continue.

Figure 3.7. Upgrade from IUCLID 5.2.x to 5.3.1


IUCLID 5.3.1 Installation
IUCLID 5
You are about to install IUCLID 5.3.1. Before continuing, please verify that the correct
version of Java is installed (6) and that the database software PostgreSQL has been installed
(version 8.4 is recommended, version 9 can now be used). See the installation manua
for descriptions of these processes.
Installed Java version is: JAVA 6
Make a fresh installation of IUCLID 5.3.1
Upgrade from IUCLID 5.3.0 to 5.3.1
Upgrade from IUCLID 5.2.x to 5.3.1
Continue
Cancel

The next screen provides some reminders about the overall process of upgrading from IUCLID 5.2.x, as shown below.

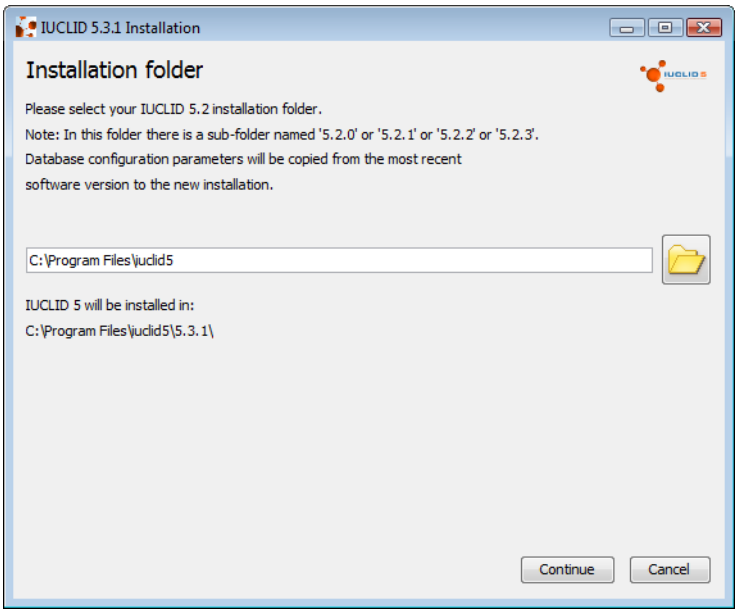
Figure 3.8. Upgrade from IUCLID 5.2.x to 5.3.1 - Reminder


IUCLID 5.3.1 Installation
The upgrade process from IUCLID 5.2 to IUCLID 5.3.1 must be carried out in three steps:
1) Back-up the database. Use the built-in back-up functionality of IUCLID, and/or the back-up function of PostgreSQL.
2) Run the installer, select the upgrade option and proceed with the installation.
3) Run the migration tool.
This screen is at the start of part (2). Therefore, you should already have backed-up your database. Please confirm that that has been done, before proceeding with the installation of IUCLID 5.3.1. After performing the installation, the migration tool can be run, whenever it is convenient. IUCLID 5.3.1 cannot be started until the migration tool has been run.
continue
cancel

3.2.3. Destination folder for the installation

In the second step of the installer, either enter the path or browse for, the parent folder of your current IUCLID 5.2 installation. This is the folder you previously selected to install IUCLID 5.2. In this folder you should have at least one folder named `5.2.x` that was created automatically during a previous installation process. The installer reads the file system and automatically selects the folder for the most recent version of IUCLID it finds. During the installation it will read the database configuration parameters from that folder. When you click Continue, the installer will create the folder that is stated directly underneath the folder selection field, then copy the old database configuration parameters and the new software into it. In the screenshot shown below, the value for the new folder is `C:\Program Files\iuclid5\5.3.1\`.

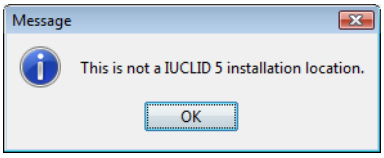
Figure 3.9. Installation folder


IUCLID 5.3.1 Installation
Installation folder
Please select your IUCLID 5.2 installation folder.
Note: In this folder there is a sub-folder named '5.2.0' or '5.2.1' or '5.2.2' or '5.2.3'.
Database configuration parameters will be copied from the most recent
software version to the new installation.
C:\Program Files\iuclid5
IUCLID 5 will be installed in:
C:\Program Files\iuclid5\5.3.1\
Continue
Cancel

When you are sure that the values are correct, click Continue.

The following error message is displayed, if the destination folder does not contain a previous installation of IUCLID 5.2.

Figure 3.10. Incorrect destination folder

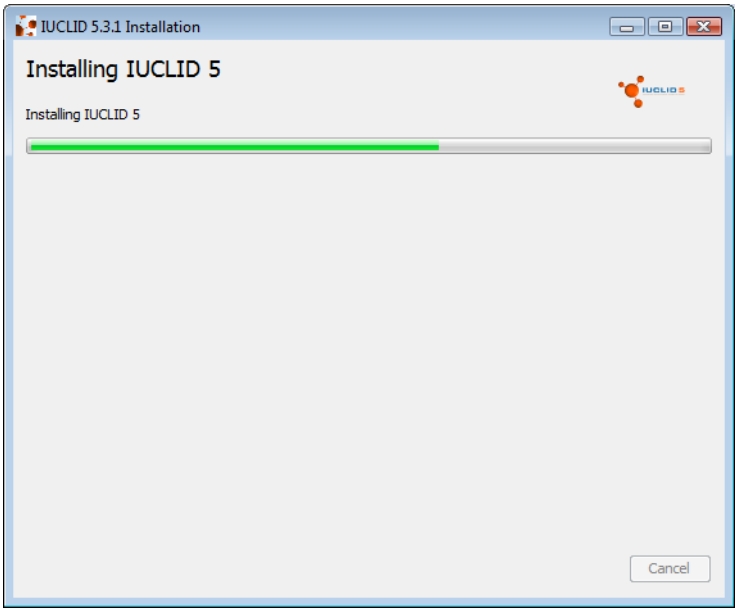


If either of the two error messages *Cannot create destination folder* or *Access denied* are given, for a possible solution, see Appendix A, *Tips on launching the installer and access rights* later in this document.

3.2.4. Installation of IUCLID 5.3.1 application files

After choosing the folder where IUCLID 5.2 was previously installed and clicking Continue, the installer will install automatically IUCLID 5.3.1 in a subfolder of the same installation folder and will name this new subfolder `5.3.1`. The actual installation process will take a few seconds.

Figure 3.11. Installing IUCLID 5



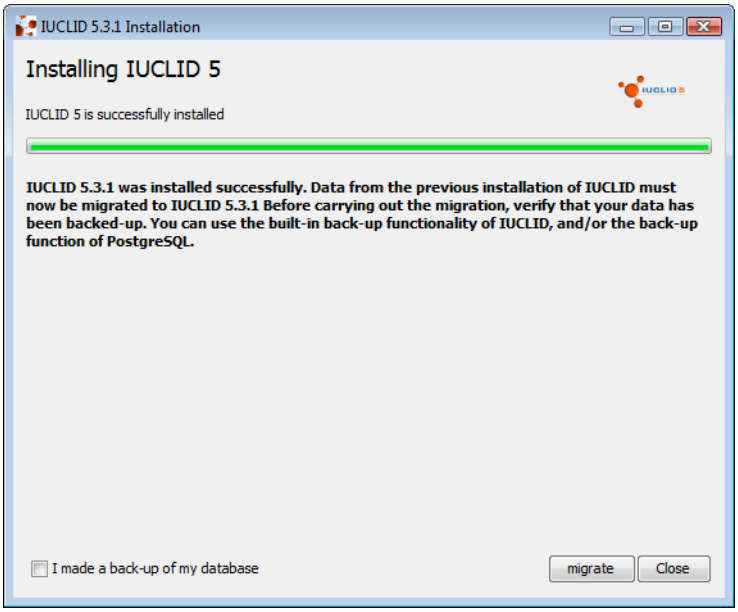
During the installation process, the following operations are performed:

- The new versions of the application files are copied to the installation folder of the new version.
- Plugins that had been installed in the previous version of IUCLID 5, are copied over to the new version of IUCLID 5, but only if they are compatible with the new version. The installer automatically detects whether a plugin is compatible. If a plugin is no longer visible in the user interface of IUCLID 5 after upgrading, visit the IUCLID web site at http://iuclid.eu to see whether a compatible version is available.
- The configuration files for the previous installation are copied to the new installation.
- A shortcut to IUCLID 5 is created on the desktop of the Windows account under which the installation is performed, as shown below.

Figure 3.12. Shortcut to IUCLID 5

After a successful installation, the following screen is shown.

Figure 3.13. IUCLID 5.3.1 is installed successfully

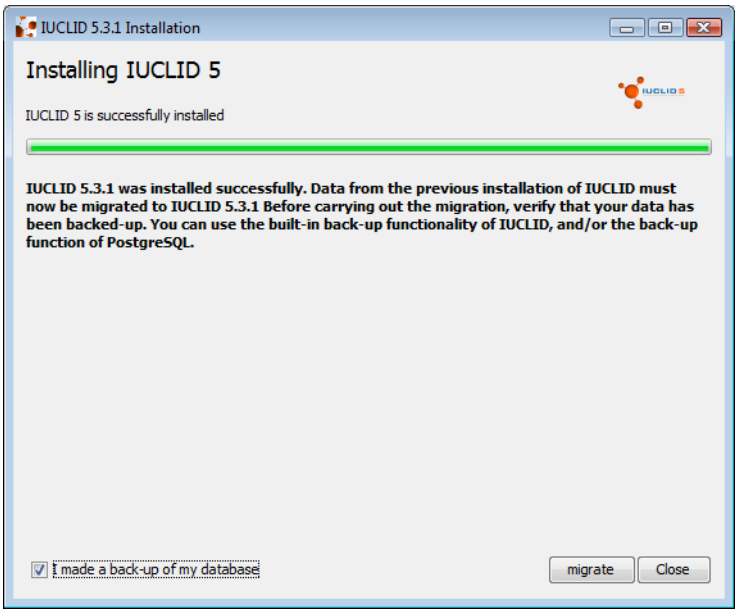

IUCLID 5.3.1 Installation
Installing IUCLID 5
IUCLID 5 is successfully installed
IUCLID 5.3.1 was installed successfully. Data from the previous installation of IUCLID must now be migrated to IUCLID 5.3.1 Before carrying out the migration, verify that your data has been backed-up. You can use the built-in back-up functionality of IUCLID, and/or the back-up function of PostgreSQL.
I made a back-up of my database
migrate
Close

This page contains advice about backing up your database and a button that starts the migration process. At this point you can choose to either begin the migration process now, by clicking *migrate*, or to do it later by clicking close.

3.2.5. The migration tool

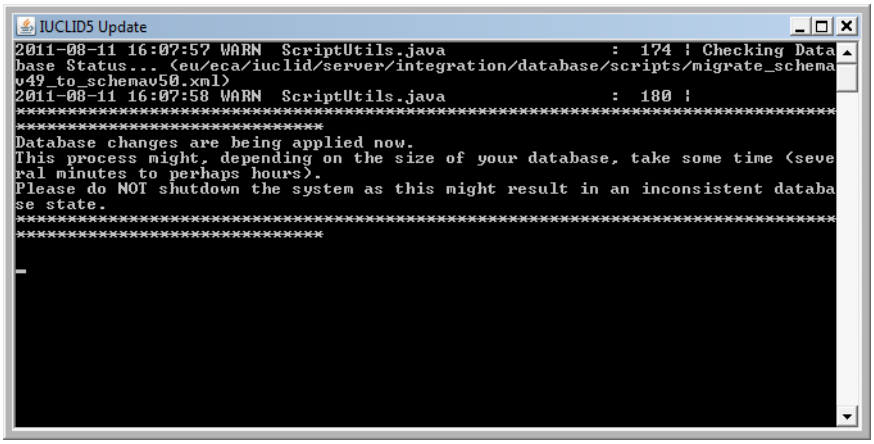
There are two ways to perform the migration. One is to run the script named `update.bat` that was installed along with IUCLID 5.3.1. It is in the installation folder. The other is to start migration from the last page of the installer. This is done by ticking the box labelled I made a back-up of my database, then clicking the button named *migrate*.

Figure 3.14. IUCLID 5.3.1 is installed successfully - upgrade


IUCLID 5.3.1 Installation
Installing IUCLID 5
IUCLID 5 is successfully installed
IUCLID 5.3.1 was installed successfully. Data from the previous installation of IUCLID must now be migrated to IUCLID 5.3.1 Before carrying out the migration, verify that your data has been backed-up. You can use the built-in back-up functionality of IUCLID, and/or the back-up function of PostgreSQL.
I made a back-up of my database
migrate
Close

Whilst the migration tool is running, a window is shown for the program *cmd* that contains a terminal to the command line of Windows. A typical example is shown in the screen shot below:

Figure 3.15. Migration tool is running


IUCLID5 Update
2011-08-11 16:07:57 WARN ScriptUtils.java : 174 ! Checking Database Status... (eu/eca/iuclid/server/integration/database/scripts/migrate_schemav49_to_schemav50.xml)
2011-08-11 16:07:58 WARN ScriptUtils.java : 180 !
Database changes are being applied now.
This process might, depending on the size of your database, take some time (several minutes to perhaps hours).
Please do NOT shutdown the system as this might result in an inconsistent database state.

Do not allow anything to happen that might interrupt this process. Do not close the window. When the process has finished, the message *Database update successfully finished* is displayed in the window briefly, before the window closes automatically. If the process does become interrupted, try starting again from the beginning. If that does not work, restore the original 5.2 database from a back-up, and try again.

3.2.6. Starting IUCLID 5

If the migration tool has run successfully, you can now launch the newly installed IUCLID 5.3. Launch IUCLID 5 by double-clicking the icon that the installer created on your Desktop, as shown below. It is also possible to launch IUCLID 5 by running the file `iuclid5.cmd` that is included in the installation directory. The initialisation process is not required. All of the data that was present in the upgraded system should be present in the new system. Therefore, it should be possible to log in to any of the user accounts from the previous system.

Figure 3.16. Shortcut to IUCLID 5

3.3. Upgrading from IUCLID 5.0 / 5.1 to IUCLID 5.3

Important

There is no automatic upgrade of the database from IUCLID 5.0 / 5.1 to IUCLID 5.3. The data must be transferred manually from the old to the new database as described in the sub-section below.

Each installation of IUCLID 5 must have its own database.

3.3.1. Migration of data to IUCLID 5.3 from a previous version

Before starting to install IUCLID 5.3, all the data must be exported from the old IUCLID 5 using the Back-up plugin that is available on the IUCLID web site. The export process is essential because the exported data will later be imported into IUCLID 5.3. When it is run, the Back-up plugin asks the user to create and enter a single password. This will become the password for all the user accounts in the new installation. An exception is the account *SuperUser* which has a default password of *root*. To import the exported data into IUCLID 5.3, use the built-in Restore feature of IUCLID 5.3 that can be found from the menu File / Administrative tools. This feature allows the upload of data that was exported using the Back-up plugin on the old version of IUCLID 5.

3.3.2. Database configuration for running IUCLID 5.3 and a previous version at the same time

If you already have a previous version of IUCLID 5, it is recommended to keep it for the time being. It can be deleted in the future when you are absolutely sure that it is no longer needed. What follows is some information and advice as to how you can manage more than one version of IUCLID 5. As stated above, each installation of IUCLID 5 must have its own database. A new database must be created for IUCLID 5.3 because the structure of the database differs from that of previous versions. This requirement can be met in a variety of different ways. The following sub-sections describe two common sets of circumstances. The database for IUCLID 5.3 can be run on the same instance of the database software as a previous version of IUCLID 5, however, it must have a unique name within that instance of the database software. When IUCLID 5.3 is run for the first time on an empty database, it will automatically create all the correct tables and the initialisation wizard will start.

3.3.3. IUCLID 5.0 / 5.1 was installed using the setup-kit

The IUCLID 5 set-up kit included the database software PostgresSQL. The set-up kit installed the PostgreSQL database software, the IUCLID 5 software, and stored the database data, all under the same folder named IUCLID. The set-up kit created installations of IUCLID 5 that run PostgreSQL on a non-standard port (5433). Therefore, if an installation of IUCLID 5.3 is made with an independent installation of PostgreSQL running on the standard port (5432), it is possible to run it at the same time as an installation that was made with the set-up kit. For example, if IUCLID 5.3 is installed using the installer according to its instructions and with default settings, the new installation can be run at the same time as a previous installation that was made with the set-up kit.

3.3.4. IUCLID 5.0 / 5.1 was installed manually

In this case, you will already have an installation of PostgreSQL that is independent of IUCLID, and a database for use with IUCLID 5.0 / 5.1. There is no need to install PostgreSQL again, although you might want to take this opportunity to upgrade to PostgreSQL 9. There can be more than one database running on a single instance of the database software. Therefore, to be

able to run IUCLID 5.3 and a previous version at the same time, create a new empty database for IUCLID 5.3. The name of the new database must be unique within that instance of the database software.

Chapter 4. Initialisation of an installation of IUCLID 5

This chapter describes the configuration that is required to create a working IUCLID 5 system from an installation of IUCLID 5 that has an empty database. There are two scenarios: either to create a working installation from scratch, or to load data from a back-up that was made using the built-in back-up function of IUCLID. During initialisation from scratch, reference substance data and a legal entity are uploaded into the database, and the required user accounts can be created. For initialisation from back-up, make sure that the back-up files are accessible from the system on which IUCLID will be initialised. What to do in each scenario is described in the rest of this chapter.

4.1. Starting IUCLID 5

Launch IUCLID 5 by double-clicking the icon that the installer created on your Desktop, as shown below. It is also possible to launch IUCLID 5 by running the file `iuclid5.cmd` that is included in the installation directory.

Figure 4.1. Shortcut to IUCLID 5

4.2. First steps wizard

When you start IUCLID 5 for the first time, the *First steps* wizard is run automatically. It guides you through the steps required to make a working user account and to upload the data required to use IUCLID 5 in a practical setting. The settings that relate to user accounts can also be changed after having run the wizard, using the features described in the IUCLID 5 User Manual.

Important

This wizard allows a single user account to be created, per run. This user is in addition to the *SuperUser* account that comes with the installation. It is essential to have at least one user account in addition to *SuperUser* because *SuperUser* should be used only for the special tasks that only it can carry out. See the IUCLID 5 User Manual for more detail.

As part of the First steps wizard, a legal entity must be uploaded into the IUCLID 5 installation in the form of a LEOX file. Therefore, before running this wizard, make sure that a LEOX file for the legal entity of your company or organisation is accessible to your computer. For more information, see the IUCLID 5 User Manual.

The First steps wizard provides the option of uploading the following information to your IUCLID 5 installation. For details, see the IUCLID 5 User Manual:

- EC Inventory
- Inventory of Reference substances

Although these uploads are optional, it is strongly recommended to do them during the first run of the First steps wizard. To do so, you will need to have the data accessible to your computer whilst running this wizard.

The First steps wizard can be run at any time, but only by the *SuperUser*. This is done from the file menu within IUCLID 5 **Administrative tools** / **Initialise**.

When starting the IUCLID 5 for the first time, the only user available is an administrator named *SuperUser*. Log in as *SuperUser* by entering the following case-sensitive values into the login screen as shown below:

Username: SuperUser

Password: root

The First steps wizard then proceeds. Each page of the wizard is described in a figure below.

Figure 4.2. Step 1 of the First steps wizard - Introduction

The wizard presents some useful information. There are no actions other than to read the information. Click the **Next** button.

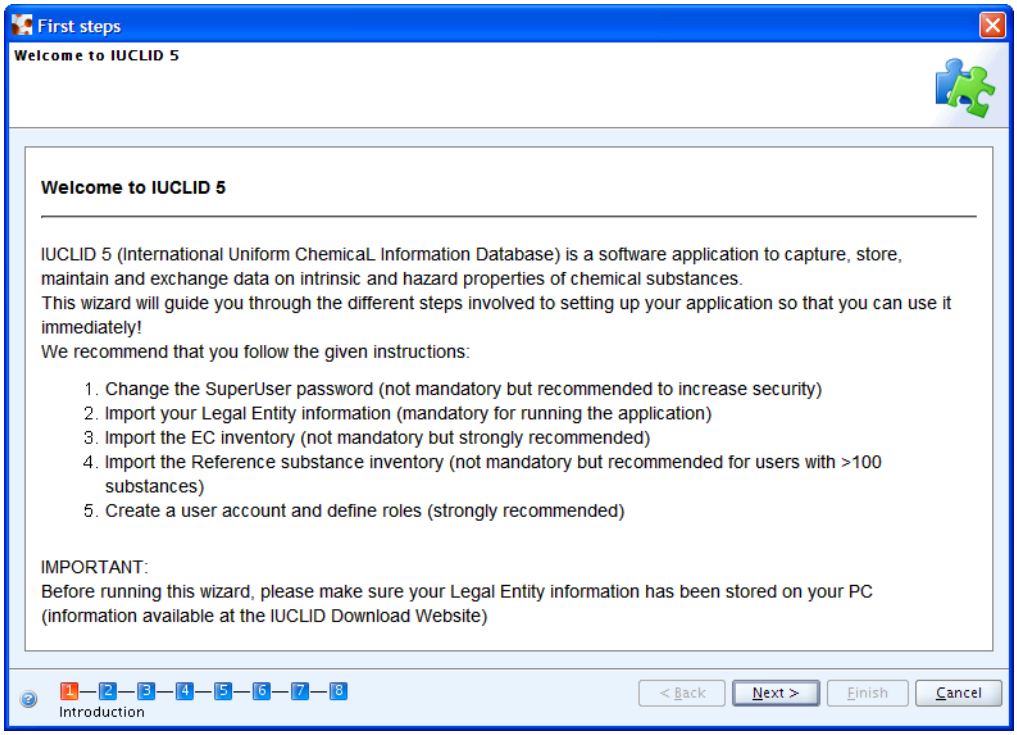

First steps
Welcome to IUCLID 5
Welcome to IUCLID 5
IUCLID 5 (International Uniform ChemicaL Information Database) is a software application to capture, store, maintain and exchange data on intrinsic and hazard properties of chemical substances.
This wizard will guide you through the different steps involved to setting up your application so that you can use it immediately!
We recommend that you follow the given instructions:
1. Change the SuperUser password (not mandatory but recommended to increase security)
2. Import your Legal Entity information (mandatory for running the application)
3. Import the EC inventory (not mandatory but strongly recommended)
4. Import the Reference substance inventory (not mandatory but recommended for users with >100 substances)
5. Create a user account and define roles (strongly recommended)
IMPORTANT:
Before running this wizard, please make sure your Legal Entity information has been stored on your PC (information available at the IUCLID Download Website)
1 2 3 4 5 6 7 8
Introduction
< Back
Next >
Finish
Cancel

Figure 4.3. Step 2 of the First steps wizard - Init mode - New installation

To initialise a new database, select the button `New Installation`as shown below and continue to the next step.

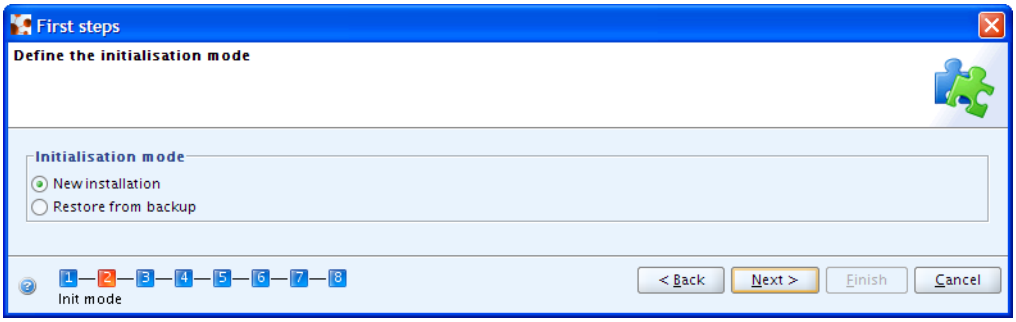
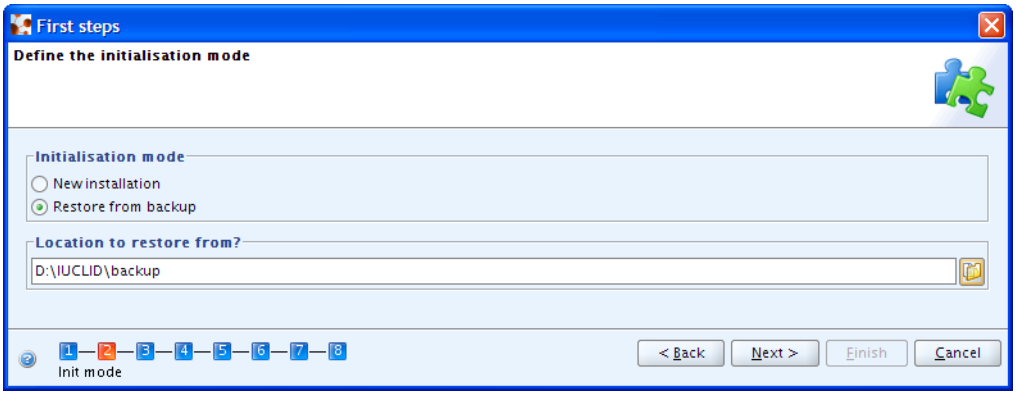


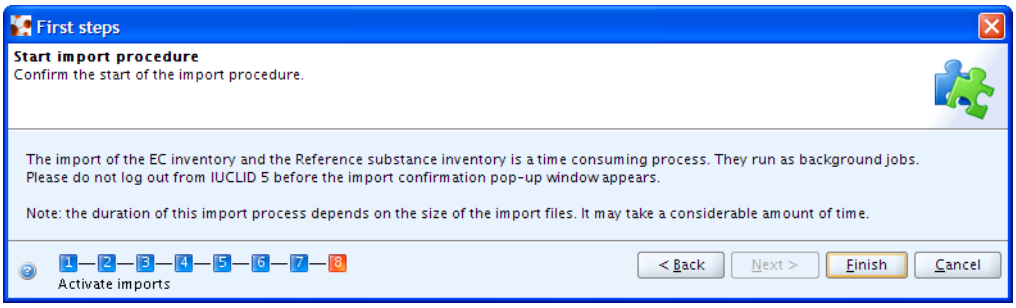
Figure 4.4. Step 2 of the First steps wizard - Init mode - Restore from backup

To restore from a backup of a previous version of IUCLID 5, select the button `Restore from backup` then enter the directory containing the backup files as shown in the example below.



Click **Next**. The wizard jumps to its last step, where the importation of data is started, as shown below.

Figure 4.5. Restoration from a back-up - Step 8 - Activate imports


First steps
Start import procedure
Confirm the start of the import procedure.
The import of the EC inventory and the Reference substance inventory is a time consuming process. They run as background jobs.
Please do not log out from IUCLID 5 before the import confirmation pop-up window appears.
Note: the duration of this import process depends on the size of the import files. It may take a considerable amount of time.
1 2 3 4 5 6 7 8
Activate imports
< Back
Next >
Finish
Cancel

The import may take some time. Click *Finish*. When the restoration is complete, the following screen is shown.

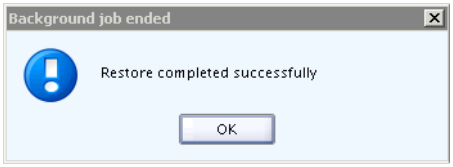


Figure 4.6. Step 3 of the First steps wizard - Change password

If you have not yet changed the default password of the *SuperUser* to a more secure value than *root*, the traffic light in the wizard screen will be yellow. To change the password, check the box `Change SuperUser password` , enter the old password *root* and then enter the new password. After confirming the password, click the button **Next**.

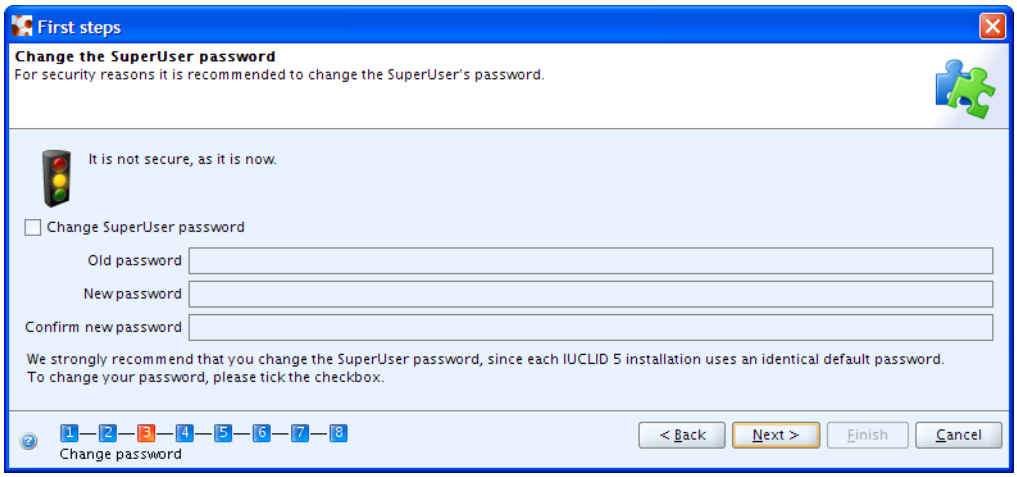
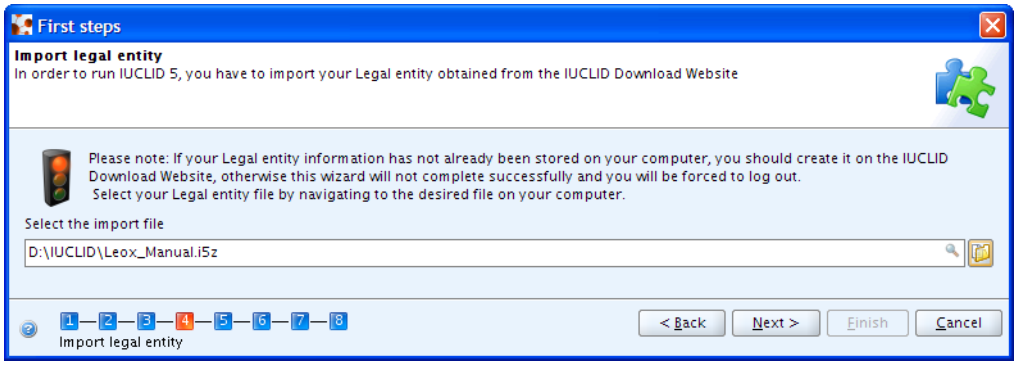
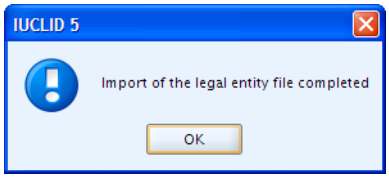

First steps
Change the SuperUser password
For security reasons it is recommended to change the SuperUser's password.
It is not secure, as it is now.
Change SuperUser password
Old password
New password
Confirm new password
We strongly recommend that you change the SuperUser password, since each IUCLID 5 installation uses an identical default password.
To change your password, please tick the checkbox.
1 2 3 4 5 6 7 8
Change password
< Back
Next >
Finish
Cancel

Figure 4.7. Step 4 of the First steps wizard - Import Legal Entity

To import a Legal entity (see the IUCLID 5 User Manual) select its LEOX file by browsing to the file. The browsing is accessed by clicking on the folder icon to the right of the field Select the import file. Click the **Next** button. The Legal entity is imported immediately.


First steps
Import legal entity
In order to run IUCLID 5, you have to import your Legal entity obtained from the IUCLID Download Website
Please note: If your Legal entity information has not already been stored on your computer, you should create it on the IUCLID Download Website, otherwise this wizard will not complete successfully and you will be forced to log out.
Select your Legal entity file by navigating to the desired file on your computer.
Select the import file
D:\IUCLID\Leox_Manual.i5z
1 2 3 4 5 6 7 8
Import legal entity
< Back
Next >
Finish
Cancel



Important

You must import at least one Legal entity in order to succeed with this wizard. If you have no Legal entity in the IUCLID 5 system, the traffic light in the wizard screen will be red. The First steps wizard will be automatically launched when you log in to IUCLID 5 until a Legal entity has been successfully imported.

Figure 4.8. Step 5 of the First steps wizard - Import EC Inventory

EC inventory import - To import the EC inventory, select the file for the EC inventory (see the IUCLID 5 User Manual). The EC Inventory will not be imported immediately. The import will start at the end of the First steps wizard. Depending on your machine speed and the size of the inventory, this import can take some time, e.g. up to half an hour.

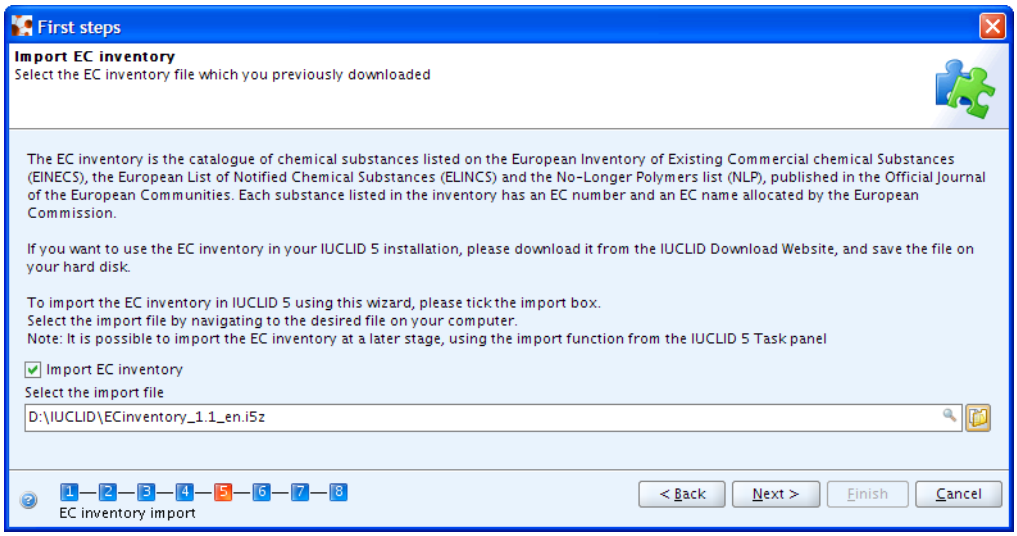
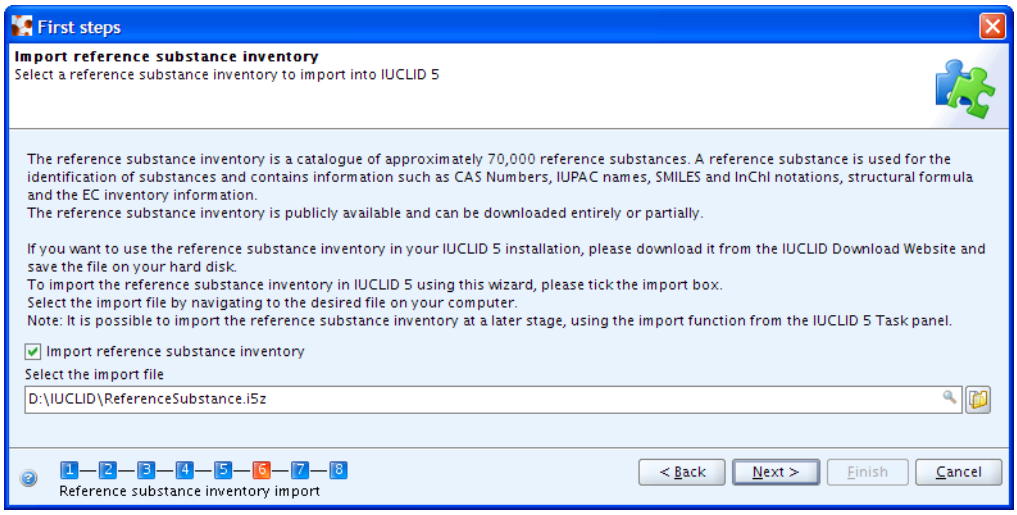

First steps
Import EC inventory
Select the EC inventory file which you previously downloaded
The EC inventory is the catalogue of chemical substances listed on the European Inventory of Existing Commercial chemical Substances (EINECS), the European List of Notified Chemical Substances (ELINCS) and the No-Longer Polymers list (NLP), published in the Official Journal of the European Communities. Each substance listed in the inventory has an EC number and an EC name allocated by the European Commission.
If you want to use the EC inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website, and save the file on your hard disk.
To import the EC inventory in IUCLID 5 using this wizard, please tick the import box.
Select the import file by navigating to the desired file on your computer.
Note: It is possible to import the EC inventory at a later stage, using the import function from the IUCLID 5 Task panel
Import EC inventory
Select the import file
D:\IUCLID\ECinventory_1.1_en.i5z
1 2 3 4 5 6 7 8
EC inventory import
< Back
Next >
Finish
Cancel

Figure 4.9. Step 6 of the First steps wizard - Import reference substance inventory

Reference substance inventory import - Select the file for the Reference substance inventory (see the IUCLID 5 User Manual). The Reference substance inventory will not be imported immediately. The import will start at the end of the first steps wizard together with the EC Inventory import. Depending on your machine speed and the size of the inventory, this bulk operation may take a long time. The import of the Reference substance inventory itself can take **up to several hours**.

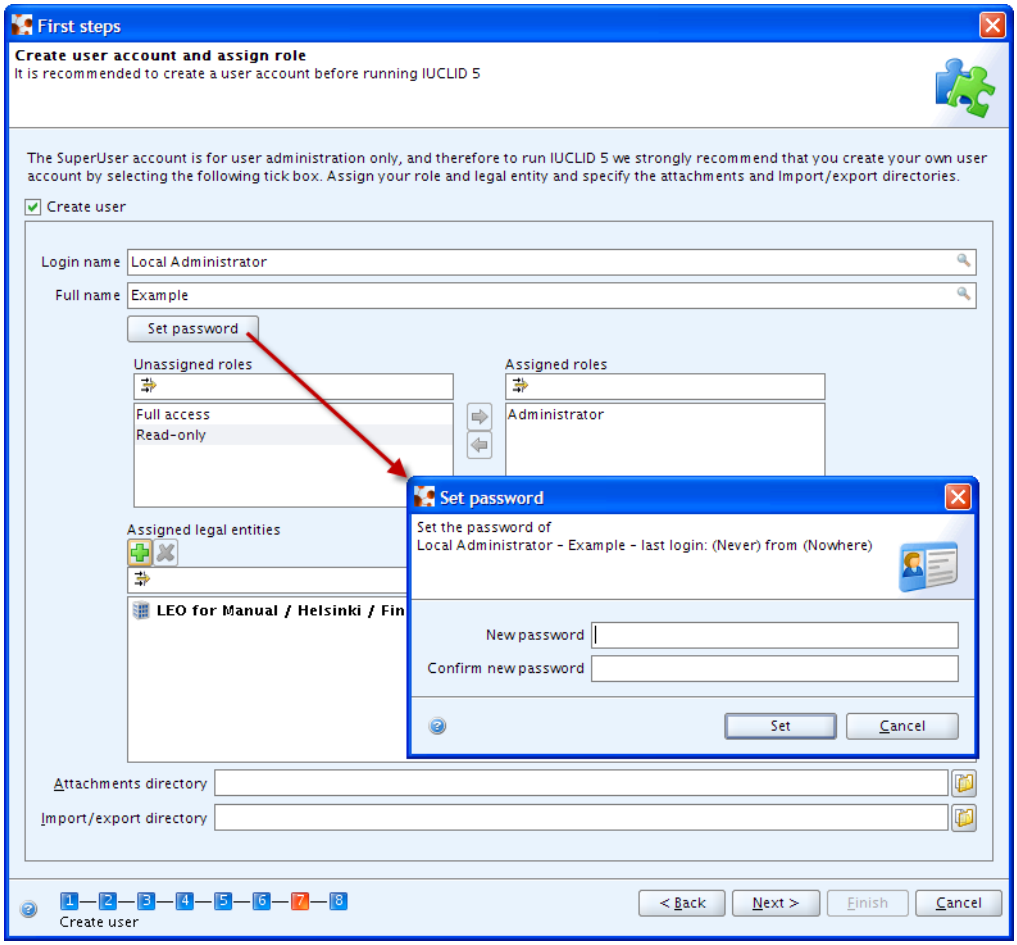

First steps
Import reference substance inventory
Select a reference substance inventory to import into IUCLID 5
The reference substance inventory is a catalogue of approximately 70,000 reference substances. A reference substance is used for the identification of substances and contains information such as CAS Numbers, IUPAC names, SMILES and InChI notations, structural formula and the EC inventory information.
The reference substance inventory is publicly available and can be downloaded entirely or partially.
If you want to use the reference substance inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website and save the file on your hard disk.
To import the reference substance inventory in IUCLID 5 using this wizard, please tick the import box.
Select the import file by navigating to the desired file on your computer.
Note: It is possible to import the reference substance inventory at a later stage, using the import function from the IUCLID 5 Task panel.
Import reference substance inventory
Select the import file
D:\IUCLID\ReferenceSubstance.i5z
1 2 3 4 5 6 7 8
Reference substance inventory import
< Back
Next >
Finish
Cancel

Tip

Time and IT resources can be saved by importing into IUCLID only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set*, a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

Figure 4.10. Step 7 of the First steps wizard - Create user account and assign role

Create a new user account and define its user access rights by assigning it a role. It is essential to create a new user because general working within IUCLID 5 with the SuperUser is not supported. Only one user can be created per run of the First steps wizard.


First steps
Create user account and assign role
It is recommended to create a user account before running IUCLID 5
The SuperUser account is for user administration only, and therefore to run IUCLID 5 we strongly recommend that you create your own user account by selecting the following tick box. Assign your role and legal entity and specify the attachments and Import/export directories.
Create user
Login name
Local Administrator
Full name
Example
Set password
Unassigned roles
Full access
Read-only
Assigned roles
Administrator
Assigned legal entities
LEO for Manual / Helsinki / Fin
Set password
Set the password of
Local Administrator - Example - last login: (Never) from (Nowhere)
New password
Confirm new password
Set
Cancel
Attachments directory
Import/export directory
1 2 3 4 5 6 7 8
Create user
< Back
Next >
Finish
Cancel

- Select the checkbox `Create user`.

  Fill in all the fields. The user needs a `Login name` for identification during login. The `Full name` is used for proper user identification. The `Assigned role` is needed to administrate the access permissions. In a newly installed IUCLID 5, the roles *Administrator*, *Full access* and *Read-only* are provided by default.

- Enter a `Login name`, as it should be used for identification during login, and the `Full name` used for proper user identification.

- Optionally, click Set password and define a password.

- Click and highlight a role in the list of unassigned roles and assign it to the user by clicking the Right arrow. Assigning a Role is needed to administrate the access permissions (in a newly installed IUCLID 5, the roles *Administrator*, *Full access* and *Read-only* are provided by default).

Tip

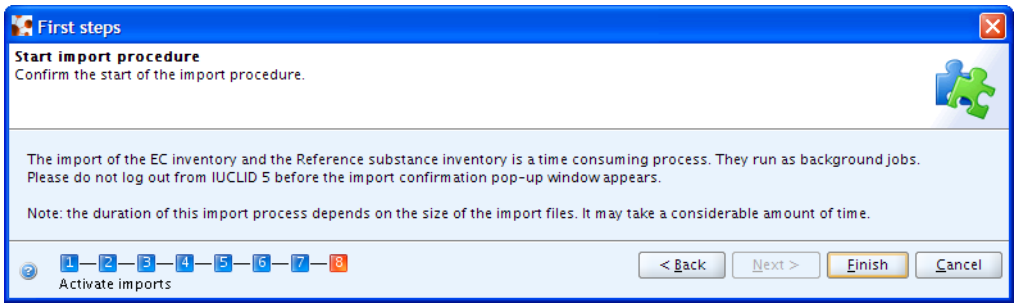
It is recommended to create a user with the *Administrator* Role regardless of whether a stand alone or a distributed version of IUCLID 5 is set up. Once a user has been created, the IUCLID 5 administrator (in case of a distributed version) can define different other user(s) and assign different role(s) to them (see the IUCLID 5 User Manual).

- Assign a Legal entity (normally the Legal entity imported in the third step of this wizard) by clicking the green plus button and performing a search for the desired Legal entity. In the Query field `Legal entity name`, enter the name of the desired Legal entity or an asterisk (*) as wildcard and click the **Search** button. In the Query results list, click the desired entry and then click the **Assign** button.
- Optionally, select default attachment and import/export directories. These settings can be changed at a later stage, as described in the IUCLID 5 User Manual.
- Click the **Next** button

Figure 4.11. Step 8 of the First steps wizard - Start import procedure

If you have selected an EC Inventory and/or Reference substances inventory file(s) during the wizard steps, you can now run the imports. Click the button **Execute imports**. Note again that these imports can take up to several hours, depending on your machine speed and the amount of data you are importing.

Then click the button **Finish**. If you have launched any imports, you will now have to wait until the imports are completed. Afterwards, you should log out and then log in again as a user for the newly defined account. Remember: general working as SuperUser is not supported.


First steps
Start import procedure
Confirm the start of the import procedure.
The import of the EC inventory and the Reference substance inventory is a time consuming process. They run as background jobs.
Please do not log out from IUCLID 5 before the import confirmation pop-up window appears.
Note: the duration of this import process depends on the size of the import files. It may take a considerable amount of time.
1 2 3 4 5 6 7 8
Activate imports
< Back
Next >
Finish
Cancel

4.3. User management

The installation of IUCLID 5 is now ready for hand-over to whoever will be maintaining the system and whoever will be managing the user accounts. The management of user accounts and their roles is described in the IUCLID 5 User Manual.

Chapter 5. Un-installation of IUCLID 5

The un-installation of IUCLID is a manual process. IUCLID can be un-installed by deleting the files that were copied to the destination machine, and reversing any changes made during the installation process. For more details about the actions that might be required, see the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.

Appendix A. Tips on launching the installer and access rights

If the installer does not launch on double clicking it, one reason could be that Windows associates the file extension jar, with some application other than Java. To get around this, launch the installer with an explicit instruction to use Java, as described in below. If required, there are more detailed step by step instructions given later in this Appendix.

Force installer to be opened by Java

1. Open a terminal in Windows that gives access to the command line.
2. Change to the directory in which the installer file is located.
3. Enter the command **java -jar iuclid5_istall.jar**

If during the installation, Windows displays error messages of the types shown below, and/or the desktop shortcut is not created, the installer had insufficient access rights.

Error message: **Cannot create the destination folder**

Error message: **C:\Program Files\iuclid\5.2.x\iuclid5.ico (Access is denied)**

If the shortcut was not created automatically, but the installation was a success, it is recommended to create the shortcut manually, rather than re-install with different access rights. The manual creation is described below.

Three ways to obtain the correct access rights

1. Run the installer from the command line. This is described in a dedicated section below.
2. Select a destination folder to which the installer has write access, i.e. replace the default value `C:Program Files/iuclid5` with something suitable on your system.
3. If you have access to a user account of type *built-in user*, log in to it and start the installer by double-clicking on the file `iuclid5_install.jar`.

To run from the command line

1. Log on as a user that has administrator rights.
2. Open the application *Command Prompt* using the option *Run as administrator*.
3. Enter the administrator password when prompted.
4. In the *Command Prompt* window, move to the folder that contains the installer Java file.
5. Enter the name of the Java file then press the key *Enter*.

Extra detail about the command line

1. #### Getting the command line

   a. Click on the *Start* icon at the bottom left of the Windows Desktop

   b. Select from the menu *All Programs / Accessories*

c. Right-click on the application *Command Prompt* then select *Run as administrator*

2. **Moving to the correct directory**

   a. to view the content of the current directory, enter the command *dir*

   b. to change to a particular drive, enter its drive letter followed by a colon, e.g. *G:*

   c. to enter a folder, enter the command *cd* followed by the directory name, e.g. *cd Documents*

   d. to go one level up in the file system, enter the command *cd ..*

Manual creation of the shortcut

1. Right-click on the Windows desktop and select the menu item *New Shortcut*.
2. Enter the location or *Browse* to the file named `iuclid5.cmd` that is included in the installation directory.
3. Enter a name for the shortcut then click *Finish*.
4. To attach a IUCLID 5 icon to the shortcut, right-click the shortcut and select *Properties*.
5. Select *Change Icon* then *Browse* to the installation directory and select the file `iuclid5.ico`. Click *Apply* and *OK* where appropriate.

If you are still having problems with the installation, before contacting the IUCLID Helpdesk, please try the FAQ located on the IUCLID web site http://iuclid.eu.